Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry

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Work-in-progress Report – *Period from 03/31/03 to 03/31/04*

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Project Summary

The present project is a multi-institution collaborative effort aimed at adapting a high-fidelity turbulent reacting flow solver called S3D to terascale, massively parallel, computer technology. S3D adopts the direct numerical simulation (DNS) approach: DNS is a unique tool in combustion science proposed to produce both high-fidelity observations of the micro-physics found in turbulent reacting flows as well as the reduced model descriptions needed in macro-scale simulations of engineering-level systems. The new S3D software is enhanced with new numerical and physical modeling capabilities; it is also modified to become object-oriented and fit into an advanced software environment based on an adaptive mesh refinement framework called GrACE and the Common Component Architecture (CCA).

Program Scope

Direct numerical simulation (DNS) is a mature and productive research tool in combustion science that is based on first principles of continuum mechanics. Because of its high demand for computational power, current state-of-the-art DNS remains limited to small computational domains (*i.e.* weakly turbulent flows) and to simplified problems corresponding to adiabatic, non-sooting, gaseous flames in simple geometries. The objective of this research project is to use terascale technology to overcome many of the current DNS limitations and allow for first-principles simulations of pollutant emissions (NO_x, soot) from turbulent combustion systems.

The effort leverages an existing DNS capability, named S3D, developed at Sandia National Laboratories. S3D is a compressible Navier-Stokes solver coupled with an integrator for detailed chemistry (CHEMKIN-compatible), and is based on high-order finite differencing, high-order explicit time integration, conventional structured meshing, and MPI-based parallel computing implementation. The objective here is to both re-design S3D for effective use on terascale high-performance computing platforms, and to enhance the code with new numerical and physical modeling capabilities.

The list of new numerical developments includes: an implicit/explicit operator-splitting technique for efficient time integration; a modified inflow boundary scheme for acoustically-smooth turbulence forcing; and a pseudo-compressibility method for more efficient computation of slow flow problems. The list of new physical modeling developments includes: a thermal radiation capability; a soot formation capability; and a Lagrangian particles capability to simulate dilute liquid fuel sprays.

The new S3D software has also been modified to fit into GrACE, an advanced parallel computing framework targeted for adaptive mesh refinement applications. Our project has developed a library of wrappers to fit the S3D Fortran 90 environment into the C++ GrACE framework. Our effort is now focused in making S3D compliant to a software interoperability standard, the Common Component Architecture (CCA) developed by the SciDAC ISIC in Ref. [1]. The CCA environment will allow exchanging software components developed by different teams working on complementary tasks. It will allow in particular the re-use of components developed by a separate Sandia-led research project called CFRFS [2]. This exchange of software components between different projects is a unique feature allowed by the SciDAC structure that promotes interactions between different teams of application scientists (our project and CFRFS [2]) and between application scientists and computer scientists (our project, CFRFS and the CCA ISIC [1]).

Recent Progress

As explained above, the present developments for S3D include a complete software re-design, new numerical methods and new physical modeling capabilities. We present here a summary of progress made during the past 12 months work period of this project extending from 03/31/02 to 03/31/03.

Software design developments:

- S3D has been modified to fit into GrACE. The developments include a new library of wrappers to fit the S3D Fortran 90 environment into the C++ GrACE framework (PSC/Roberto Gomez, Raghurama Reddy, Junwoo Lim).
- S3D is currently being adapted to the CCA framework (PSC/Raghurama Reddy)

Numerical developments:

- A new pseudo-compressibility method has been developed and implemented into S3D (UMD/Arnaud Trouvé, [3-5]). This method allows for more efficient computations of slow flow problems while still using a fully compressible formulation.
- The S3D inflow boundary scheme (using a characteristic-based analysis) has been modified to allow for injection of laminar/turbulent flow perturbations while minimizing spurious acoustic wave reflections (UMI/Hong Im, [6-8]).

Physical model developments:

- A new thermal radiation solver (discrete ordinate method, DOM, grey and non-scattering medium) has been implemented into S3D (UMI/Hong Im, [9]). A second separate solver based on the discrete transfer method (DTM) has been implemented into S3D (UMD/Arnaud Trouvé).

- A phenomenological soot model based on transport equations for the soot volume fraction and particle number density has been implemented into S3D (UMD/Arnaud Trouvé [9]).

- A Lagrangian particle model to describe dilute liquid sprays has been developed and coupled to the gas-phase Eulerian solver in S3D (UWI/Christopher Rutland, [10-12]).

New combustion science:

The new DNS solver is currently used in a series of demonstration studies selected for both their technical challenge and scientific value. The list of ongoing pilot studies includes: the simulation of turbulent ethylene-air counter-flow diffusion flames (to study flame extinction phenomena and edge-flame dynamics) [6,9,13]; the simulation of a turbulent ethylene-air jet diffusion flame near a solid wall (to study flame-wall interactions and the associated wall heat transfer) (see Fig. 1); the simulation of turbulent auto-ignition for a population of vaporizing liquid fuel (n-heptane) droplets (to study spray auto-ignition in homogeneous charge compression ignition – HCCI – engines) [10-12,14-15]. Additional S3D-based studies may be found in Refs. [16-19].

Future Plans

The main focus of the coming work period will be to: (1) release a CCA/GrACE-based version of S3D; (2) and exchange software components with the CFRFS project [2], and thereby initiate developments to adapt S3D to AMR.

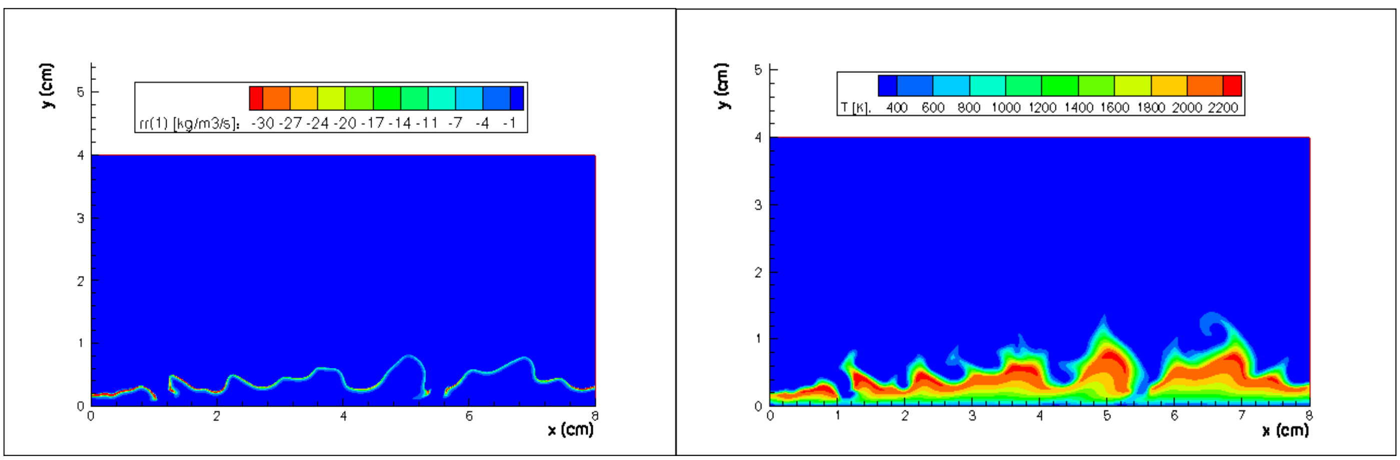

Figure 1. Instantaneous variations of fuel mass reaction rate (left) and temperature (right) during the simulation of a turbulent reacting wall boundary layer. The flow is from left to right; the flame develops at the interface of the fuel stream (bottom left) and the air stream (top left). The wall boundary (bottom) remains at 300 K. Two wall-induced flame extinction events are observed in these snapshots, near x = 1.2 cm and x = 5.4 cm.

References

[1] Armstrong, R. C., *et al.* "Center for Component Technology for Terascale Simulation Software", SciDAC Integrated Software Infrastructure Center (ISIC), http://www.cca-forum.org/ccttss/

[2] Najm, H., *et al.* "A Computational Facility for Reacting Flow Science", SciDAC project, http://cfrfs.ca.sandia.gov/

[3] Wang, Y. & Trouvé, A. (2003) “Artificial Acoustic Stiffness Reduction in Fully Compressible, Direct Numerical Simulation of Combustion”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.

[4] Wang, Y. & Trouvé, A. (2003) “Artificial acoustic stiffness reduction in fully compressible, direct numerical simulation of combustion”, *submitted to Combust. Theory Modelling*.

[5] Trouvé A., Wang Y., Im H. G., Yoo C. S., Rutland C. J., Wang Y., Chen J. H., Sutherland J. C., and Mason S. D. (2004), “Direct numerical simulation of turbulent combustion using a fully compressible flow formulation,” *10th SIAM Intl. Conf. on Numerical Combustion*, Sedona, AZ.

[6] Yoo, C. & Im, H. G. (2003) “A Computational Study on the Dynamics of Counterflow Hydrogen-Air Edge Flames”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.

[7] Yoo, C. S. and Im, H. G. (2004), “Soft inflow boundary conditions for direct numerical simulations of compressible reacting flows,” *10th SIAM Intl. Conf. on Numerical Combustion*, Sedona, AZ.

[8] Yoo, C. S. and Im, H. G. (2004), “Soft inflow boundary conditions for direct numerical simulations of compressible reacting flows,” *submitted to J. Comp. Phys*.

[9] Yoo, C. S., Im, H. G. Trouvé, A., and Wang, Y. (2004), “Direct numerical simulation of turbulent nonpremixed counterflow ethylene-air flame with soot and radiation models,” *10th SIAM Intl. Conf. on Numerical Combustion*, Sedona, AZ.

[10] Wang, Y. and Rutland, C. J. (2003), “Direct numerical simulation of turbulent droplets flow with evaporation,” *The 41st AIAA Aerospace Sciences Meeting and Exhibit*, AIAA Paper 2003-1281, 6-9 January 2003, Reno, Nevada, USA.

[11] Wang, Y. and Rutland, C. J. (2003), “On the combustion of normal heptane fuel droplets in isotropic turbulence with DNS,” *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

[12] Wang, Y. and Rutland, C. J. (2004), “Effects of temperature and equivalence ratio on the ignition of n-heptane fuel droplets in turbulent flow,” *submitted to 31st Intl. Symp. Combustion.*

[13] Yoo, C. S. and Im, H (2004), “Transient dynamics of edge flames in a laminar nonpremixed hydrogen-air counterflow,” *submitted to 31st Intl. Symp. Combustion*.

[14] Sankaran, R., Im, H. G., Hawkes, E. R. & Chen, J. H. (2004), “The effects of nonuniform temperature distribution on the ignition of a lean homogeneous hydrogen-air mixture,” *submitted to 31st Intl. Symp. Combustion*.

[15] Chen, J. H., Hawkes, E. Hewson, J. C., Sankaran, R., Im, H. G., Mason, S. D. (2004), “Ignition front propagation in a constant volume with temperature inhomogeneities,” *submitted to 31st Intl. Symp. Combustion*.

[16] Chen, J. H., Mason, S. D. & Hewson, J. C. (2003) “The Effect of Temperature Inhomogeneity on Low-Temperature Autoignition of Fuel-Lean Premixed Hydrogen/Air Mixtures”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.

[17] Hawkes, E. R. & Chen, J. H. (2003) “Turbulent Stretch Effects on Hydrogen Enriched Lean Premixed Methane-Air Flames”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.

[18] Liu, S. & & Chen, J. H. (2003) “The Effect of Product Gas Enrichment on the Chemical Response of Premixed Diluted Methane/Air Flames”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.

[19] Sutherland, J. C., Smith, P. J. & Chen, J. H. (2003) “DNS of a Nonpremixed CO-H2 Jet using Detailed Chemistry – Toward Improved LES Models”, *3rd Joint Meeting US Sections of Combustion Institute*, Chicago, IL.